Supporting Information

Remote Substituent Effects on the Oxymercuration

of 2-Substituted Norbornenes:

An Experimental and Theoretical Study.

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- **Experimental procedures for preparation of substituted norbornenes and their oxymercuration reactions (p.S2-p.S19)**
- **Cartesian coordinates (in Å) and total energies (in a.u.) predicted theoretically for the structures in Figures 4 to 8 (p.S20-p.S51)**
- **[1]H and [13]C NMR Spectra of new compounds that <u>do not</u> have elemental analytical data (Compounds: 6a, 6e, 6f, 6g, 7a, 7e, 12f/13f and 12g/13g) (p.S52-p.S59)**

(59 pages)

Experimental procedures for preparation of substituted norbornenes and their oxymercuration reactions

General Information: All reactions were carried out in an atmosphere of dry nitrogen at ambient temperature unless otherwise stated. Standard column chromatography was performed on 230-400 mesh silica gel (obtained from Silicycle) by use of flash column chromatography techniques.[32] Analytical thin-layer chromatography (TLC) was conducted on Merck precoated silica gel 60 F_{254} plates. All glassware was flame dried under an inert atmosphere of dry nitrogen. Infrared spectra were taken on a Bomem MB-100 FTIR spectrophotometer. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker-400 spectrometer. Chemical shifts for ^{1}H NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard (chloroform: δ 7.26). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard (deuterochloroform: δ 77.0). High resolution mass spectra were done by Mass Spectrometry Laboratory Services Division at the University of Guelph or by McMaster Regional Centre for Mass Spectrometry at McMaster University, Hamilton, Ontario. Elemental analyses were performed by Canadian Microanalytical Service Ltd., British Columbia or by Quantitative Technologies Inc., New Jersey.

Materials: Unless stated otherwise, commercial reagents were used without purification. Solvents were purified by distillation under dry nitrogen: from CaH_2 (CH_2Cl_2, 1,2-dichloroethane, DMF, hexanes, pyridine); from 4 Å molecular sieves (acetonitrile); from sodium (toluene, DME); from potassium/benzophenone (THF); and from sodium/benzophenone (Et_2O). Norbornenes **6b** and **7b** were prepared by literature procedures.[17] Norbornenes **6c**, **6d**, **6h**, **7c**, **7d** and **7f** are known compounds and a detailed procedure for their preparation can be found in Supporting Information.

[32] Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923.

Part I–Synthesis of Norbornenes 6a, 6e, 6f, 6g, 7a and 7e:

***Exo*-(Bicyclo[2.2.1]hept-5-en-2-yl)methyl *tert*-butyldimethylsilyl ether (6a).** *Exo*-norbornene **6b**[17a] (292 mg, 1.92 mmol) in THF (2 mL) was added via a cannula to a flame-dried flask containing $LiAlH_4$ (140 mg, 3.69 mmol) in THF (3 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 1 h and at room temperature for 5 h. After quenching with saturated NH_4Cl (5 mL), the aqueous layer was extracted with diethyl ether (4×20 mL) and the combined organic layers were washed with brine (20 mL), and dried (Na_2SO_4). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give *exo*-(bicyclo[2.2.1]hept-5-en-2-yl)methanol (210 mg, 1.69 mmol, 88%) as a colorless oil. Spectral data of this alcohol is identical to that reported in the literature.[15,33]

tert-Butyldimethylsilyl chloride (243 mg, 1.61 mmol) was added to a flame-dried flask containing the above alcohol (145 mg, 1.17 mmol) and imidazole (118 mg, 1.73 mmol) in DMF (2 mL) and the reaction was stirred for 4 h. After quenching with water (3 mL), the reaction mixture was extracted into CH_2Cl_2:hexanes (1:9) (4×20 mL), and the combined organic layers were washed with water (20 mL), brine (20 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (hexanes) to give **6a** (240 mg, 1.01 mmol, 86%) as a colorless oil: R_f 0.35 (hexanes); IR (neat): 3061 (w), 2957 (s), 2929 (s), 2885 (m), 2858 (s), 1472 (m), 1463 (m), 1384 (w), 1361 (w), 1339 (w), 1255 (s), 1187 (w), 1159 (w), 1162 (s), 1075 (s), 1006 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 6.10 (dd, 1H, J = 5.7, 3.1 Hz), 6.05 (dd, 1H, J = 5.6, 2.9 Hz), 3.70 (dd, 1H, J = 10.2, 6.0 Hz), 3.47 (dd, 1H, J = 10.0, 9.1 Hz), 2.78 (br. s, 1H), 2.75 (br. s, 1H), 1.59 (m, 1H), 1.30 (m, 2H), 1.18 (dd, 1H, J = 11.6, 8.4 Hz), 1.06 (dt, 1H, J = 11.6, 4.1 Hz), 0.91 (s, 9H), 0.058 (s, 3H), 0.056 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.74, 136.67, 67.5, 44.8, 43.3, 41.6, 41.5, 29.2, 26.0, 18.4, -5.2. HRMS calcd. for $C_{14}H_{26}SiO$: m/z 238.1753, found m/z 238.1755.

[33] Fisher, W.; Grob, C. A.; Sprecher, G.; Waldner, A. *Helv. Chim. Acta* **1980**, *63*, 928.

***Exo*-(Bicyclo[2.2.1]hept-5-en-2-yl) *tert*-butyldimethylsliyl ether (6e).** *tert*-Butyldimethylsilyl chloride (570 mg, 3.78 mmol) was added to a flame-dried flask containing alcohol **6c** (340 mg, 3.09 mmol) and imidazole (301 mg, 4.42 mmol) in DMF (4 mL) and the reaction mixture was stirred for 12 h. After quenching with water (10 mL), the reaction mixture was extracted into CH_2Cl_2:hexanes (1:9) (4×10 mL), and the combined extracts were washed with water (10 mL), brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (hexanes) to give **6e** (550 mg, 2.45 mmol, 79%) as a colorless oil: R_f 65 (hexanes); IR (neat): 3064 (w), 2957 (s), 2931 (s), 2898 (m), 2857 (s), 1473 (m), 1463 (m), 1389 (w), 1362 (m), 1332 (m), 1256 (s), 1174 (m), 1156 (w), 1102 (s), 1080 (s), 1007 (s) cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 6.15 (dd, 1H, J = 5.7, 2.9 Hz), 5.92 (dd, 1H, J = 5.7, 3.2 Hz), 3.81 (d, 1H, J = 5.5 Hz), 2.76 (br. s, 1H), 2.61 (br. s, 1H), 1.77 (d, 1H, J = 8.1 Hz), 1.57-1.49 (m, 2H), 1.25 (ddd, 1H J = 11.5, 3.5, 1.9 Hz), 0.89 (s, 9H), 0.05 (s, 3H), 0.04 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.5, 133.4, 72.7, 50.4, 45.8, 40.6, 37.4, 25.9, 18.1, -4.6, -4.7. HRMS calcd. for $C_{13}H_{24}SiO$: m/z 224.1596, found m/z 224.1600.

***Exo*-Bicyclo[2.2.1]hept-5-en-2-yl benzoate (6f).** Benzoyl chloride (0.24 mL, 2.07 mmol) was added to a flame-dried flask containing alcohol **6c** (130 mg, 1.18 mmol) and pyridine (0.30 mL, 3.71 mmol) in CH_2Cl_2 (2.5 mL) and the reaction mixture was stirred at room temperature for 12 h. After quenching with water (3 mL), the reaction mixture was extracted into CH_2Cl_2 (3×10 mL), and the combined extracts were washed with saturated $CuSO_4$ (10 mL), water (10 mL), brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:9) to give **6f** (220 mg, 1.03 mmol, 87%) as a colorless oil: R_f 0.20 (EtOAc:hexanes=1:9); IR (CH_2Cl_2): 3063 (m), 2979 (s), 2944 (m), 1717 (s), 1603 (w), 1451 (w), 1357 (w), 1332 (m), 1314 (m), 1274 (s) cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.04 (dm, 2H, J = 7.1 Hz), 7.54 (tm, 1H, J = 7.3 Hz), 7.42 (t, 2H, J = 7.7 Hz), 6.28 (dd, 1H, J = 5.7, 2.9 Hz), 6.03 (dd, 1H, J = 5.7, 3.2 Hz), 4.92 (dd, 1H, J = 6.9, 0.7 Hz), 3.03 (br. s, 1H), 2.90 (br. s, 1H), 1.82 (ddd, 1H, J = 12.6, 6.9, 2.6 Hz), 1.80 (d, 1H, J = 8.6 Hz), 1.65 (d, 1H, J = 8.6 Hz), 1.58 (dt, 1H, J = 12.6, 3.0 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.5, 141.2, 132.7, 132.5, 130.6, 129.4, 128.2, 75.7, 47.3, 46.3, 40.6, 34.7. HRMS calcd. for $C_{14}H_{14}O_2$: m/z 214.0994, found m/z 214.0988.

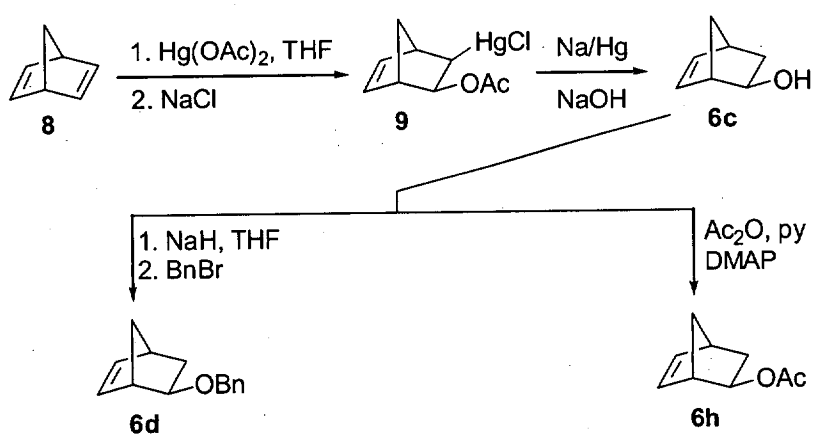
***Exo*-Bicyclo[2.2.1]hept-5-en-2-yl *p*-nitrobenzoate (6g).** *p*-Nitrobenzoyl chloride (380 mg, 2.08 mmol) was added to a flame-dried flask containing alcohol **6c** (141 mg, 1.28 mmol) and pyridine (0.30 mL, 3.71 mmol) in CH_2Cl_2 (2.5 mL) and the reaction mixture was stirred at room temperature for 12 h. After quenching with water (3 mL), the reaction mixture was extracted into CH_2Cl_2 (3×10 mL), and the combined extracts were washed with saturated $CuSO_4$ (10 mL), water (10 mL), brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give **6g** (303 mg, 1.17 mmol, 91%) as a colorless oil: R_f 0.65 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 3058 (m), 2983 (s), 2945 (m), 2871 (w), 1719 (s), 1609 (m), 1529 (s), 1507 (w), 1490 (w), 1458 (m), 1442 (w), 1320 (m), 1275 (s) cm^{-1}. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, 2H, J = 8.8 Hz), 8.19 (d, 2H, J = 8.8 Hz), 6.31 (dd, 1H, J = 5.7, 2.9 Hz), 6.03 (dd, 1H, J = 5.7, 3.2 Hz), 4.94 (d, 1H, J = 6.9 Hz), 3.05 (br. s, 1H), 2.94 (br. s, 1H), 1.85 (ddd, 1H, J = 12.7, 6.9, 2.6 Hz), 1.76 (d, 1H, J = 8.6 Hz), 1.67 (dd, 1H, J = 8.6, 0.8 Hz), 1.59 (dt, 1H, J = 12.7, 3.0 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.3, 150.2, 141.2, 135.8, 132.2, 130.3, 123.2, 76.7, 47.2, 46.2, 40.5, 34.5. HRMS calcd. for $C_{14}H_{13}NO_4$: m/z 259.0845, found m/z 259.0851.

***Endo*-(Bicyclo[2.2.1]hept-5-en-2-yl)methyl *tert*-butyldimethylsilyl ether (7a).** *Endo*-Norbornene **7b**[17b,c] (3.05 g, 20.0 mmol) in THF (15 mL) was added via a cannula to a flame-dried flask containing $LiAlH_4$ (1.52 g, 40.1 mmol) in THF (30 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 1 h. After quenching with saturated NH_4Cl (5 mL), saturated potassium/sodium tartrate (10 mL) and water (100 mL), the aqueous layer was extracted with diethyl ether (4×50 mL) and the combined organic layers were washed with brine (50 mL), and dried (Na_2SO_4). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give *endo*-(bicyclo[2.2.1]hept-5-en-2-yl)methanol (1.12 g, 9.03 mmol, 45%) as a colorless oil. Spectral data of this alcohol is identical to that reported in the literature.[33]

tert-Butyldimethylsilyl chloride (478 mg, 3.17 mmol) was added to a flame-dried flask containing the above alcohol (283 mg, 2.28 mmol) and imidazole (227 mg, 3.33 mmol) in DMF (5 mL) and the reaction was stirred for 2 h. After quenching with water (20 mL), the reaction mixture was extracted into CH_2Cl_2:hexanes (1:9) (4×10 mL), and the combined organic layers were washed with water (20 mL), brine (20 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (hexanes) to give **7a** (454 mg, 1.90 mmol, 83%) as a colorless oil: R_f 0.22 (hexanes); IR (neat) 3061 (w), 2957 (s), 2857 (s), 1472 (m), 1386 (w), 1361 (w), 1347 (w), 1255 (s), 1150 (w), 1097 (s), 1054 (m), 1006 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.11 (dd, 1H, J = 5.7, 3.0 Hz), 5.93 (dd, 1H, J = 5.7, 2.9 Hz), 3.37 (dd, 1H, J = 9.9, 6.2 Hz), 3.12 (t, 1H J = 9.6 Hz), 2.92 (br. s, 1H), 2.76 (br. s, 1H), 2.27 (m, 1H), 1.76 (ddd, 1H, J = 11.6, 9.2, 3.8 Hz), 1.41 (dd, 1H, J = 8.1, 2.0 Hz), 1.23 (d, 1H, J = 8.1 Hz), 0.89 (s, 9H), 0.43 (ddd, 1H, J = 11.6, 4.5, 2.6 Hz), 0.03 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.0, 132.5, 66.5, 49.3, 43.6, 42.2, 41.6, 28.7, 26.0, 18.3, -5.27, -5.34. HRMS calcd. for $C_{14}H_{26}SiO$: m/z 238.1753, found m/z 238.1753.

***Endo*-(bicyclo[2.2.1]hept-5-en-2-yl) *tert*-butyldimethylsilyl ether (7e).** *tert*-Butyldimethylsilyl chloride (622 mg, 4.13 mmol) was added to a flame-dried flask containing alcohol **7c** (191 mg, 1.73 mmol) and imidazole (179 mg, 2.63 mmol) in DMF (2.2 mL) and the reaction was stirred for 22 h. After quenching with water (5 mL), the reaction mixture was extracted into CH_2Cl_2:hexanes (1:9) (4×5 mL), and the combined organic layers were washed with water (10 mL), brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:19) to give **7e** (151 mg, 0.673 mmol, 39%) as a colorless oil: R_f 0.31 (hexanes); IR (neat): 3070 (m), 2957 (s), 2931 (s), 2886 (s), 2858 (s), 1472 (m), 1463 (m), 1368 (m), 1256 (s), 1161 (m), 1123 (s), 1103 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.29 (dd, 1H, *J* = 5.6, 3.0 Hz), 5.96 (dd, 1H, *J* = 5.6, 2.9 Hz), 4.45 (dt, 1H, *J* = 7.9, 3.2 Hz), 2.85 (br. s, 1H), 2.74 (m, 1H), 1.93 (ddd, 1H, *J* = 15.6, 7.9, 3.8 Hz), 1.35 (m, 1H), 1.20 (d, 1H, *J* = 8.2 Hz), 0.85 (s, 9H), 0.77 (dt, 1H, *J* = 11.9, 3.2 Hz), 0.04 (s, 3H), 0.03 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.5, 132.0, 72.7, 48.5, 47.2, 42.6, 37.1, 25.9, 18.1, -4.6, -4.7. HRMS calcd. for $C_{13}H_{24}SiO$: m/z 224.1596, found m/z 224.1598.

Part II–Synthesis of Norbornenes 6c, 6d and 6h:



(2-Acetoxy-*cis-exo*-bicyclo[2.2.1]hept-5-en-3-yl)mercuric chloride (9). $Hg(OAc)_2$ (10.4 g, 32.6 mmol) was slowly added (over 45 min.) to a flame-dried flask containing norbornadiene **8** (5.39 mL, 50.0 mmol) in THF (25 mL). The mixture was stirred at room temperature for 12 h, quenched with NaCl (14.6 g, 25.0 mmol) and stirred for 30 min. After quenching with water, the aqueous layer was extracted into CH_2Cl_2, and the combined organic layers were washed with brine and dried ($MgSO_4$). Rotary evaporation and recrystallization from hot EtOAc yielded the product **9** as white crystals (9.57 g, 24.7 mmol, 76%). Spectral data identical to those reported in the literature.[34]

***Exo*-Bicyclo[2.2.1]hept-5-en-2-ol (6c).** Sodium amalgam (6%w/w Na/Hg, 92.7 g) was added to a flame-dried flask containing mercuric chloride **9** (7.64 g, 19.7 mmol) in NaOH (2.5M, 200 mL) and the reaction mixture was stirred for 18 h. The reaction was quenched with water (200 mL),

[34] Kitching, W.; Atkins, A. R.; Wickham, G.; Alberts, V. *J. Org. Chem.* **1981**, *46*, 563.

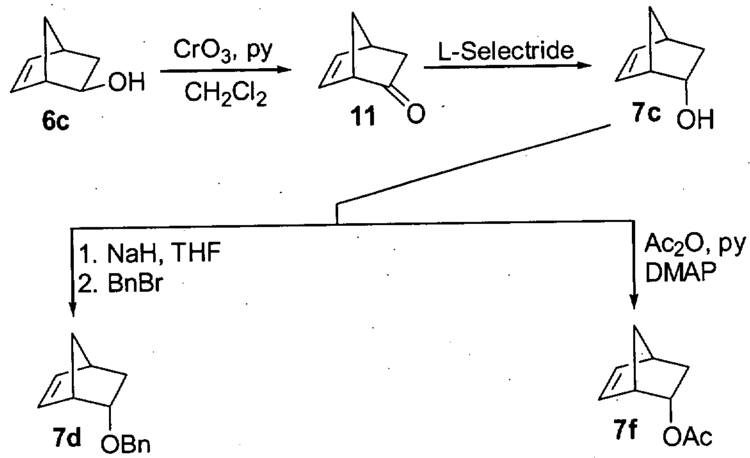
extracted into diethyl ether (4 × 200 mL), and the combined organic layers were washed with water (200 mL), brine (200 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give **6c** (1.63 g, 14.8 mmol, 75%) as soft white crystals. Spectral data identical to those reported in the literature.[35,36]

***Exo*-Benzyl(bicyclo[2.2.1]hept-5-en-2-yl) ether (6d).** Alcohol **6c** (410 mg, 3.72 mmol) in THF (2 mL) was added via a cannula to a flame-dried flask containing pentane-washed sodium hydride (134 mg, 5.58 mmol) in THF (2 mL) at 0 °C. The reaction mixture stirred at 50 °C for 3 h. After cooling the reaction mixture to room temperature, benzyl bromide (1.32 mL, 11.1 mmol) was added and the reaction mixture was stirred for 12 h. After quenching with aqueous NH_4Cl (5 mL), the reaction mixture was extracted into diethyl ether (4 × 10 mL), washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:9) to give **6d** (538 mg, 2.69 mmol, 73%) as a colorless oil. Spectral data identical to those reported in the literature.[35]

***Exo*-Bicyclo[2.2.1]hept-5-en-2-yl acetate (6h).** Acetic anhydride (0.91 mL, 9.64 mmol) was added to a flame-dried flask containing alcohol **6c** (667 mg, 6.05 mmol), pyridine (1.53 mL, 18.9 mmol) and dimethylaminopyridine (2 crystals) in CH_2Cl_2 (12 mL). The reaction mixture was stirred for 24 h. After quenching with water (10 mL), the aqueous layer was extracted with CH_2Cl_2 (4×40 mL) and the combined organic layers were washed with saturated $CuSO_4$ (10 mL), water (10 mL), brine (10 mL), and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:19) to give **6h** (777 mg, 5.10 mmol, 84%) as a colorless oil. Spectral data identical to those reported in the literature.[37,38]

[35] Arjona, O.; Fernandez de la Pradilla, R.; Plumet, J.; Viso, A. *J. Org. Chem.* **1991**, *56*, 6227.
[36] Fischer, W.; Grob, C. A.; Sprecher, G.; Waldner, A. *Helv. Chim. Acta* **1980**, *63*, 816.
[37] Oberhauser, Th.; Bodenteich, M.; Faber, K.; Penn, G.; and Griengl, H. *Tetrahedron* **1987**, *43*, 3931.

Part III–Synthesis of Norbornenes 7c, 7d and 7f:



Bicyclo[2.2.1]hept-5-en-2-one (11). Alcohol **6c** (8.44 g, 76.6 mmol) in CH_2Cl_2 (250 mL) was added via a cannula to a flame-dried flask containing CrO_3 (47.2 g, 472 mmol) and pyridine (76 mL, 945 mmol) in CH_2Cl_2 (600 mL) and the reaction mixture was stirred for 48 h. The reaction mixture was filtered through a short plug of silica (eluted with CH_2Cl_2) and the organic layer was washed with 5% KOH, 5% HCl, saturated $NaHCO_3$, saturated NaCl, and dried (Na_2SO_4). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give ketone **11** (3.95 g, 36.5 mmol, 48%) as white solids. Spectral data identical to those reported in the literature.[39]

***Endo*-Bicyclo[2.2.1]hept-5-en-2-ol (7c).** L-Selectride (1M in THF, 40.0 mL, 40.0 mmol) was added to a flame-dried flask containing ketone **11** (3.52 g, 32.6 mmol) in THF (35 mL) at –78 °C. The reaction mixture was stirred at –78 °C for 3 h and at –20 °C for 1 h. After quenching with water (20 mL), the aqueous layer was extracted with diethyl ether (5×30 mL) and the combined organic layers were washed with water (100 mL), brine (100 mL), and dried (Na_2SO_4). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=3:7) to give **7c** (2.76 mg, 25.0 mmol, 77%) as a colorless oil. Spectral data identical to those reported in the literature.[36]

***Endo*-Benzyl(bicyclo[2.2.1]hept-5-en-2-yl) ether (7d).** Alcohol **7c** (227 mg, 2.06 mmol) in THF (1 mL) was added via a cannula to pentane-washed sodium hydride (81.2 mg, 3.38 mmol) in THF (1 mL) at 0 °C. The reaction stirred at 40 °C for 3 h. After cooling the reaction mixture to room temperature, benzyl bromide (0.74 mL, 6.22 mmol) was added and the reaction mixture was stirred for 20 h. After quenching with aqueous NH_4Cl (10 mL), the reaction mixture

[38] Brands, K. M. J.; Kenda, A. S. *Tetrahedron Lett.* **1992**, *33*, 5887.

was extracted into ethyl acetate (4 × 5 mL), washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give **1j** (160 mg, 0.799 mmol, 39%) as a colorless oil. Spectral data identical to those reported in the literature.[35]

***Exo*-Bicyclo[2.2.1]hept-5-en-2-yl acetate (7f).** Acetic anhydride (0.20 mL, 2.1 mmol) was added to a flame-dried flask containing alcohol **7c** (154 mg, 1.40 mmol), pyridine (0.34 mL, 4.20 mmol) and dimethylaminopyridine (2 crystals) in CH_2Cl_2 (0.5 mL). The reaction mixture was stirred for 24 h. After quenching with water (5 mL), the aqueous layer was extracted with CH_2Cl_2 (4×5 mL) and the combined organic layers were washed with saturated $CuSO_4$ (5 mL), water (5 mL), brine (5 mL), and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:9) to give **7f** (78.2 mg, 0.514 mmol, 37%) as a colorless oil. Spectral data identical to those reported in the literature.[37,38]

Part IV–Oxymercuration of 2-Substituted Norbornenes:

Mercuric chlorides 12a and 13a. $Hg(OAc)_2$ (159 mg, 0.499 mmol) was added to a flame-dried flask containing norbornene **6a** (102 mg, 0.43 mmol) in THF (0.4 mL). The mixture was stirred at room temperature for 18 h, quenched with NaCl (133 mg, 2.27 mmol) and stirred for 6 h. After quenching with water (10 mL), the aqueous layer was extracted into CH_2Cl_2 (4×10 mL), and the combined organic layers were washed with brine (20 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give an inseparable mixture of **12a** and **13a** (208 mg, 0.39 mmol, 91%, **12a**:**13a**=1:1) as a white powder: R_f 0.59 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 2955 (s), 2929 (s), 2884 (s), 2857 (s), 1732 (s), 1472 (m), 1372 (m), 1316 (w), 1232 (s), 1105 (s), 1021 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 4.86 (d, 0.5H, J = 6.1 Hz), 4.84 (d, 0.5H, J = 6.0 Hz), 3.43-3.36 (m, 1.5H), 3.25 (t, 0.5H, J = 9.6 Hz), 2.72 (dd, 0.5H, J = 7.0, 2.6 Hz), 2.68 (dd, 0.5H, J = 6.8, 2.5 Hz), 2.62 (m, 0.5H), 2.57 (br. s, 0.5H), 2.44 (m, 1H), 2.04 (s, 3H), 1.58-1.50 (m, 2H), 1.34 (m, 1H), 1.31-1.23 (m, 1H), 1.19 (ddd, 0.5H, J = 12.6, 5.5, 3.8 Hz), 0.99 (dt, 0.5H, J = 13.3, 4.7 Hz), 0.885 (s, 4.5H), 0.875 (s, 4.5H),

[39] Oppolzer, W.; Chapuis, C.; Dupuis, D.; Guo, M. *Helv. Chim. Acta* **1985**, *68*, 2100.

0.038 (s, 1.5H), 0.035 (s, 1.5 H), 0.028 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 169.7, 169.6, 80.4, 80.1, 66.4, 65.7, 62.5, 62.0, 45.6, 44.8, 42.5, 42.0, 40.2, 39.0, 34.2, 33.6, 33.0, 27.5, 25.93, 25.86, 21.8, 18.3, 18.2, -5.3. Anal. Calcd. for $C_{16}H_{29}ClHgO_3Si$: C, 36.02; H, 5.48. Found C, 36.14; H, 5.46.

Mercuric chlorides 12b and 13b. $Hg(OAc)_2$ (225 mg, 0.706 mmol) was added to a flame-dried flask containing norbornene **6b** (92.4 mg, 0.607 mmol) in THF (0.61 mL). The mixture was stirred at room temperature for 18 h, quenched with NaCl (183 mg, 3.13 mmol) and stirred for 24 h. After quenching with water (5 mL), the aqueous layer was extracted into CH_2Cl_2 (4×10 mL), and the combined organic layers were washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give an inseparable mixture of **12b** and **13b** (195 mg, 0.436 mmol, 72%, **12b**:**13b**=5:1) as a white crystalline solid: R_f 0.64 (EtOAc:hexanes=2:3); IR (CH_2Cl_2): 3446 (w), 3056 (w), 2953 (s), 2882 (m), 2845 (w), 1730 (s), 1436 (s), 1372 (s), 1299 (s), 1290 (s), 1067 (m), 1020 (s); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.90 (d, 0.18H, J = 8.4 Hz), 4.88 (d, 0.82H, J = 7.2 Hz), 3.674 (s, 0.54H), 3.669 (s, 2.46H), 2.89 (s, 0.82H), 2.78 (s, 0.18H), 2.72 (dd, 0.82H, J = 6.9, 2.6 Hz), 2.68 (dd, 0.18H, J = 6.8, 2.1 Hz), 2.57 (m, 1H), 2.28 (dd, 1H, J = 8.9, 4.8 Hz), 2.06 (m, 3H), 1.96 (m, 1H), 1.60 (m, 1H), 1.50 (d, 1H, J = 9.8 Hz), 1.45 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz); major isomer (**12b**): δ 174.7, 169.5, 79.2, 61.0, 51.7, 46.8, 44.3, 42.1, 34.1, 27.9, 21.6. Visible peaks for minor isomer (**13b**): δ 169.3, 78.9, 60.8, 46.3, 40.8, 39.8, 34.8, 34.5. Anal. Calcd. for $C_{11}H_{15}ClHgO_4$: C, 29.54; H, 3.38. Found C, 29.55; H, 3.36.

Mercuric chlorides 12c and 13c. $Hg(OAc)_2$ (282 mg, 0.885 mmol) was added to a flame-dried flask containing norbornene **6c** (76.5 mg, 0.694 mmol) in THF (1 mL). The mixture was stirred at room temperature for 12 h, quenched with NaCl (270 mg, 4.62 mmol) and stirred for 30 min. After quenching with water (5 mL), the aqueous layer was extracted into CH_2Cl_2 (4×5 mL), and the combined organic layers were washed with brine (5 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=2:3) to give an inseparable mixture of **12c** and **13c** (139 mg, 0.343 mmol, 49%, **12c**:**13c**=6:1) as a white powder: R_f 0.08 (EtOAc:hexanes=2:3); IR (CH_2Cl_2): 3400 (br w), 2961 (m), 2927 (m), 1728 (s), 1372 (m), 1296 (w), 1235 (s), 1071 (m), 1021 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 4.79 (d, 0.15H, J = 7.1 Hz), 4.74 (d, 0.85H, J = 6.9 Hz), 3.86 (d, 0.15H, J = 7.3 Hz), 3.72 (d, 0.85H, J = 6.2 Hz), 2.59 (dd, 0.15H, J = 7.1, 2.6 Hz), 2.54-2.47 (m, 2.7H), 2.06 (s, 0.45H), 2.05 (s, 2.55 H), 1.72-1.58 (m, 4.15H), 1.45 (dt, 0.15H, J = 16.8, 6.8 Hz), 1.34 (ddm, 0.85H, J = 14.2, 5.3 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz) of major isomer (**12c**): δ 169.8, 79.3, 74.3, 56.0, 47.5 41.6, 36.1, 32.3, 21.7. Anal. Calcd. for $C_9H_{13}ClHgO_3$: C, 26.68; H, 3.23. Found C, 26.75; H, 3.22.

Mercuric chlorides 12d and 13d. $Hg(OAc)_2$ (580 mg, 1.82 mmol) was added to a flame-dried flask containing norbornene **6d** (306 mg, 1.53 mmol) in THF (1.5 mL). The mixture was stirred at room temperature for 18 h, quenched with NaCl (451 mg, 7.71 mmol) and stirred for 6 h. After quenching with water (10 mL), the aqueous layer was extracted into CH_2Cl_2 (4×10 mL), and the combined organic layers were washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give an inseparable mixture of **12d** and **13d** (437 mg, 0.882 mmol, 58%, **12d**:**13d**=9:1) as white crystals: R_f 0.79 (EtOAc:hexanes=2:3); IR (CH_2Cl_2): 3087 (m), 3066 (m), 3027 (m), 2973 (s), 2932 (s), 2880 (s), 2777 (w), 2951 (w), 1721 (s), 1644 (m), 1608 (m), 1496 (s), 1453 (s), 1367 (s), 1299 (s), 1236 (s), 1180 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.32 (m, 5H), 4.79 (d, 0.1H, J = 7.1 Hz), 4.75 (d, 0.9H, J = 6.9 Hz), 4.49 (d_{AB}, 1H, J = 11.9 Hz), 4.44 (d_{AB}, 1H, J = 11.9 Hz), 3.53 (m, 0.1H), 3.38 (d, 0.9H, J = 6.2 Hz), 2.73 (br. s, 0.9H), 2.71 (br. s, 0.1H), 2.68 (m, 0.1H), 2.60 (dd, 0.1H, J = 7.1, 2.6 Hz), 2.53 (d, 0.9H, J = 4.5 Hz), 2.45 (dd, 0.9H, J = 6.9, 2.4 Hz), 2.07 (s, 0.3H), 2.05 (s, 2.7H), 1.71 (ddm, 0.9H, J = 10.4, 0.8 Hz), 1.66-1.54 (m, 2.1H), 1.49 (ddd, 1H, J = 13.8, 4.9, 2.3 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz) of major isomer (**12d**): δ 169.7, 138.3, 128.4, 127.6, 127.5, 81.3, 79.6, 70.7, 56.2, 43.7, 41.3, 33.7, 32.7, 21.7. Anal. Calcd. for $C_{16}H_{19}ClHgO_3$: C, 38.79; H, 3.87. Found C, 38.72; H, 3.79.

Mercuric chlorides 12e and 13e. $Hg(OAc)_2$ (716 mg, 2.25 mmol) was added to a flame-dried flask containing norbornene **6e** (230 mg, 1.02 mmol) in THF (1 mL). The mixture was stirred at room temperature for 21 h, quenched with NaCl (278 mg, 4.75 mmol) and stirred for 2 h. After quenching with water (5 mL), the aqueous layer was extracted into CH_2Cl_2 (4×5 mL), and the combined organic layers were washed with brine (5 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:9) to give an inseparable mixture of **12e** and **13e** (439 mg, 0.845 mmol, 83%, **12e**:**13e**=12:1) as a white powder: R_f 0.67 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 2956 (s), 2931 (s), 2887 (m), 2857 (s), 1732 (s), 1472 (m), 1463 (m), 1440 (w), 1372 (m), 1318 (w), 1300 (w), 1250 (s), 1236 (s), 1175 (w), 1089 (s), 1052 (w), 1013 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 4.77 (d, 0.08H, J = 7.1 Hz), 4.71 (d, 0.92H, J = 6.8 Hz), 3.73 (d, 0.08H, J = 5.2), 3.58 (d, 0.92H, J = 6.4), 2.63 (d, 0.08H, J = 2.8 Hz), 2.59 (dd, 0.08H, J = 7.0, 2.6 Hz), 2.48-2.45 (m, 1.84H), 2.41 (br. s, 0.92H), 2.37 (br. s, 0.08H), 2.05 (s, 0.24), 2.04 (s, 2.76H), 1.72 (dm, 1H, J = 10.4 Hz), 1.55 (dm, 1H, J = 10.5 Hz), 1.51 (dd, 1H, J = 6.5, 2.0 Hz), 1.44 (m, 0.08H), 1.32 (dd, 0.92H, J = 13.0, 4.2 Hz), 0.86 (s, 9H), 0.03 (s, 3H), 0.02 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) of major isomer (**12e**): δ 169.7, 79.6, 74.5, 56.1, 47.8, 41.3, 36.9, 32.3, 25.7, 21.7, 17.9, -4.7, -4.8. Anal. Calcd. for $C_{15}H_{27}ClHgO_3Si$: C, 34.68; H, 5.24. Found C, 34.60; H, 5.26.

Mercuric chlorides 12f and 13f. $Hg(OAc)_2$ (103 mg, 0.322 mmol) was added to a flame-dried flask containing norbornene **6f** (56.2 mg, 0.262 mmol) in THF (0.5 mL). The mixture was stirred at room temperature for 72 h, quenched with NaCl (400 mg, 6.83 mmol) and stirred for 4 h. The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give an inseparable mixture of **12f** and **13f** (111 mg, 0.218 mmol, 83%, **12f**:**13f**=12:1) as a white powder: R_f 0.28 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 3054 (s), 2987 (m), 1734 (s), 1713 (s), 1653 (w), 1602 (w), 1559 (w), 1451 (m), 1422 (s), 1266 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.00 (d, 2H, J = 7.3 Hz), 7.56 (t, 1H, J = 7.2 Hz), 7.43 (t, 2H, J = 7.7 Hz), 4.99 (d, 0.076H, J = 7.1 Hz), 4.90 (dd, 0.076H, J = 6.9, 2.7 Hz), 4.84 (d, 0.924H, J = 6.9 Hz), 4.76 (dm, 0.924H, J = 5.3 Hz), 2.85 (br. s, 0.924H), 2.79 (br. s, 0.076H), 2.78 (d, 0.076H, J = 6.0 Hz), 2.72 (d, 0.076H, J = 6.9 Hz), 2.66 (d, 0.924H, J = 6.9 Hz), 2.63 (d, 0.924H, J = 4.9 Hz), 2.07 (s, 3H), 1.81 (dd, 1H, J = 14.0, 6.9 Hz), 1.73 (br. s, 2H), 1.66 (dm, 1H, J = 14.0 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz) of major isomer (**12f**): δ 169.7, 166.1, 133.1, 130.1, 129.5, 128.4, 79.1, 76.8, 55.5, 44.8, 41.5, 33.4, 33.2, 21.7.

Mercuric chlorides 12g and 13g. $Hg(OAc)_2$ (614 mg, 1.93 mmol) was added to a flame-dried flask containing norbornene **6g** (152 mg, 0.586 mmol) in THF (1 mL). The mixture was stirred at room temperature for 72 h, quenched with NaCl (700 mg, 12.0 mmol) and stirred for 4 h. The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=2:3) to give an inseparable mixture of **12g** and **13g** (240 mg, 0.433 mmol, 74%, **12g**:**13g**=14:1) as a white powder: R_f 0.50 (EtOAc:hexanes=2:3); IR (CH_2Cl_2): 3044 (s), 2977 (m), 1720 (s), 1701 (m), 1684 (w), 1653 (w), 1527 (s), 1374 (w), 1351 (w), 1279 (s), 1239 (m) cm^{-1}; ^1H NMR (d_6-DMSO, 400 MHz): δ 8.31 (d, 2H, J = 8.7 Hz), 8.15 (d, 2H, J = 8.7 Hz), 4.88 (d, 0.065H, J = 6.7 Hz), 4.86 (d, 0.065H, J = 7.2 Hz), 4.71 (d, 0.935H, J = 6.7 Hz), 4.69 (d, 0.935H, J = 7.1 Hz), 2.84 (br. s, 1H), 2.40 (m, 2H), 1.96 (s, 3H), 1.78-1.68 (m, 2H), 1.56-1.51 (m, 2H). ^{13}C NMR (d_6-DMSO, 100 MHz) of major isomer (**12g**): δ 169.4, 163.8, 150.2, 135.4, 130.6, 123.9, 78.6, 78.2, 53.2, 44.4, 41.1, 33.4, 32.9, 21.6.

Mercuric chlorides 12h and 13h. $Hg(OAc)_2$ (972 mg, 3.05 mmol) was added to a flame-dried flask containing norbornene **6h** (212 mg, 1.39 mmol) in THF (1.5 mL). The mixture was stirred at room temperature for 48 h, quenched with NaCl (413 mg, 7.06 mmol) and stirred for 24 h. After quenching with water (10 mL), the aqueous layer was extracted into CH_2Cl_2 (4×10 mL), and the combined organic layers were washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=2:3) to give an inseparable mixture of **12h** and **13h** (466 mg, 1.04 mmol, 75%, **12h**:**13h**=14:1) as a white powder: R_f 0.61 (EtOAc:hexanes=2:3); IR (CH_2Cl_2): 3056 (w), 2976 (m), 2882 (w), 1716 (s), 1462 (w), 1440 (m), 1376 (s), 1248 (s), 1179 (w), 1072 (s), 1045 (s), 1020 (s) cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 4.82 (d, 0.067H, J = 7.0 Hz), 4.70 (d, 0.933H, J = 6.9 Hz), 4.56 (d, 0.067H, J = 5.0 Hz), 4.42 (d, 0.933H, J = 6.6 Hz), 2.65 (s, 1H), 2.60 (dd, 0.067H, J = 7.0, 2.3 Hz), 2.52 (dd, 0.933H, J = 6.8, 2.2 Hz), 2.46 (d, 1H, J = 4.9 Hz), 1.98 (s, 3H), 1.93 (s, 3H), 1.64-1.59 (m, 2H), 1.51 (d, 1H, J = 10.4 Hz), 1.39 (ddm, 1H, J = 14.0, 4.8 Hz). ^{13}C ($CDCl_3$, 100 MHz) of major isomer (**12h**): δ 170.5, 169.6, 78.8, 76.2, 55.3, 44.5, 41.3, 33.2, 32.7, 21.6, 21.1. Anal. Calcd. for $C_{11}H_{15}ClHgO_4$: C, 29.54; H, 3.38. Found C, 29.63; H, 3.36.

Mercuric chlorides 14a and 15a. $Hg(OAc)_2$ (259 mg, 0.813 mmol) was added to a flame-dried flask containing norbornene **7a** (162 mg, 0.679 mmol) in THF (0.7 mL). The mixture was stirred at room temperature for 18 h, quenched with NaCl (200 mg, 3.42 mmol) and stirred for 24 h. After quenching with water (10 mL), the aqueous layer was extracted into CH_2Cl_2 (4×10 mL), and the combined organic layers were washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:9) to give an inseparable mixture of **14a** and **15a** (290 mg, 0.543 mmol, 80%, **14a**:**15a**=1:1) as a white powder: R_f 0.66 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 2955 (s), 2930 (s), 2857 (s), 1732 (s), 1471 (m), 1372 (m), 1297 (w), 1236 (s), 1092 (s), 1019 (s) cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 5.20 (d, 0.5H, J = 6.8 Hz), 4.69 (d, 0.5H, J = 7.0 Hz), 3.59-3.46 (m, 1.5H), 3.31 (t, 0.5H, J = 9.5 Hz), 3.08 (dd, 0.5H, J = 7.0, 2.6 Hz), 2.67 (dd, 0.5H, J = 6.8, 2.6 Hz), 2.65 (d, 0.5H, J = 4.8 Hz), 2.59 (d, 0.5H, J = 3.3 Hz), 2.48 (d, 0.5H, J = 4.0 Hz), 2.37 (d, 0.5H, J = 5.1 Hz), 2.02 (m, 1H), 1.99 (s, 1.5H), 1.98 (s, 1.5H), 1.70-1.63 (m, 2H), 1.36 (dm, 0.5H, J = 10.6 Hz), 1.32 (dm, 0.5H, J = 10.2 Hz), 0.83 (s, 9H), 0.82 (ddd, 0.5H, J = 12.6, 4.7, 2.8 Hz), 0.52 (ddd, 0.5H, J = 13.0, 5.7, 1.8 Hz), -0.01 (s, 3H), -0.02 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 169.5, 169.3, 80.1, 76.2, 63.5, 62.8, 55.4, 45.6, 42.9, 42.4, 41.9, 41.1, 39.3, 37.8, 33.2, 26.9, 25.8, 25.7, 21.71, 21.67, 18.1, 18.0, -5.4, -5.5, -5.6. Anal. Calcd. for $C_{16}H_{29}ClHgO_3Si$: C, 36.02; H, 5.48. Found C, 36.13; H, 5.45.

Mercuric chlorides 14b and 15b. $Hg(OAc)_2$ (760 mg, 2.38 mmol) was added to a flame-dried flask containing norbornene **7b** (308 mg, 2.02 mmol) in THF (2 mL). The mixture was stirred at room temperature for 24 h, quenched with NaCl (590 mg, 10.1 mmol) and stirred for 12 h. After quenching with water (20 mL), the aqueous layer was extracted into CH_2Cl_2 (4×10 mL), and the combined organic layers were washed with brine (20 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give an inseparable mixture of **14b** and **15b** (559 mg, 1.25 mmol, 62%, **14b**:**15b**=5:1) as white crystals: R_f 0.56 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 2962 (m), 1716 (s), 1455 (m), 1435 (m), 1373 (m), 1308 (m), 1251 (s), 1215 (s), 1126 (m), 1079 (w), 1017 (s) cm^{-1}. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.90 (d, 0.18H, J = 8.4 Hz), 4.88 (d, 0.82H, J = 7.1 Hz), 3.72 (s, 0.54H), 3.68 (s, 2.46H), 3.11 (dm, 0.18H, J = 13.7 Hz), 2.93 (m, 0.82H), 2.85-2.78 (m, 2H), 2.69 (dm, 0.18H, J = 2.8 Hz), 2.54 (d, 0.82H, J = 4.9 Hz), 2.04 (s, 2.46H), 2.03 (s, 0.54H), 1.82-1.73 (m, 2H), 1.59 (m, 0.18H), 1.55 (ddd, 0.82H, J = 13.5, 5.4, 2.3 Hz), 1.40 (dm, 1H, J = 10.3 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz); Major isomer (**14b**): δ 174.0, 169.5, 79.6, 56.6, 51.9, 45.9, 43.7, 43.2, 38.1, 26.7, 21.7. Minor isomer (**15b**): δ 174.1, 169.3, 76.6, 61.4, 51.9, 46.3, 41.7, 41.2, 38.1, 32.8, 21.7. Anal. Calcd. for $C_{11}H_{15}ClHgO_4$: C, 29.54; H, 3.38. Found C, 29.46; H, 3.39.

Mercuric chlorides 14c and 15c. $Hg(OAc)_2$ (67.2 mg, 0.211 mmol) was added to a flame-dried flask containing norbornene **7c** (7.00 mg, 0.0635 mmol) in THF (1.5 mL). The mixture was stirred at room temperature for 4 d, quenched with NaCl (18.6 mg, 0.318 mmol) and stirred for 12 h. After quenching with water (5 mL), the aqueous layer was extracted into EtOAc (4×5 mL), and the combined organic layers were washed with brine (5 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=2:3) to give an inseparable mixture of **14c** and **15c** (7.74 mg, 0.0191 mmol, 30%, **14c**:**15c**=3:1) as a white solid: R_f 0.14 (EtOAc:hexanes=2:3); IR (CH_2Cl_2): 3450 (br m), 3054 (m), 2964 (s), 1732 (s), 1446 (w), 1373 (m), 1302 (w), 1266 (s), 1237 (s), 1203 (w), 1133 (w), 1017 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 5.52 (d, 0.25H, J = 6.9 Hz), 4.92 (d, 0.75, J = 7.0 Hz), 4.34 (m, 0.25H), 4.29 (dt. 0.75H, J = 10.0, 3.9 Hz), 3.54 (dd, 0.75H, J= 7.0, 2.5 Hz), 2.96 (dd, 0.25H, J = 7.1, 2.7 Hz), 2.65 (dm, 0.25H, J = 4.8 Hz), 2.63 (m, 1H), 2.45 (d, 0.75H, J = 5.3 Hz), 2.064 (s, 0.75H), 2.060 (s, 2.25 H), 2.00 (ddd, 1H, J = 13.7, 10.0, 5.5 Hz), 1.69-1.58 (m, 2H), 1.39-1.21 (m, 1H), 0.93 (dt, 0.25H, J = 13.3, 3.4 Hz), 0.80 (dt, 0.75H, J = 13.6, 3.5 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz); Major isomer (**14c**): δ 169.5, 79.9, 71.8, 52.7, 45.7, 43.4, 35.0, 34.0, 21.7. Visible peaks for minor isomer (**15c**): δ 74.9, 69.7, 49.1, 41.6, 40.0, 36.1. Anal. Calcd. for $C_9H_{13}ClHgO_3$: C, 26.68; H, 3.23. Found C, 26.88; H, 3.32.

Mercuric chlorides 14d and 15d. $Hg(OAc)_2$ (194 mg, 0.609 mmol) was added to a flame-dried flask containing norbornene **7d** (100 mg, 0.499 mmol) in THF (0.5 mL). The mixture was stirred at room temperature for 24 h, quenched with NaCl (216 mg, 3.69 mmol) and stirred for 12 h. After quenching with water (7.5 mL), the aqueous layer was extracted into CH_2Cl_2 (4×8 mL), and the combined organic layers were washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:4) to give an inseparable mixture of **14d** and **15d** (87.9 mg, 0.177 mmol, 36%, **14d**:**15d**=6:1) as a white solid: R_f 0.33 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 3053 (w), 3026 (w), 2967 (s), 2832 (w), 2774 (w), 1699 (s), 1498 (s), 1454 (s), 1399 (m), 1345 (s), 1303 (s), 1232 (s), 1166 (m), 1137 (m), 1103 (s), 1016 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.34 (m, 5H), 5.44 (d, 0.14H J = 7.0 Hz), 4.89 (d, 0.86H, J = 6.9 Hz), 4.73 (d_{AB}, 0.14H, J = 11.1 Hz), 4.46 (d_{AB}, 0.86H, J = 12.3 Hz), 4.40 (d_{AB}, 1H, J = 11.9 Hz), 3.98 (dt, 0.14H, J = 10.3, 3.7 Hz), 3.93 (dt, 0.86H, J = 9.9, 3.8 Hz), 3.40 (dd, 0.86H, J = 7.0, 2.2 Hz), 2.90 (m, 0.28H), 2.73 (m, 0.86H), 2.61 (d, 0.14H, J = 3.6 Hz), 2.43 (d, 0.86H, J = 5.2 Hz), 2.08 (s, 0.42H), 2.04 (s, 2.58H), 1.93 (ddd, 1H, J = 13.9, 9.9, 5.4 Hz), 1.72-1.59 (m, 1H), 1.31 (d, 1H, J = 10.7 Hz), 1.04 (dt, 0.14H, J = 13.1, 3.0 Hz), 0.95 (dt, 0.86H, J = 13.7, 3.5 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz); Major isomer (**14d**): δ 169.6, 138.2, 128.4, 127.82, 127.76, 80.0, 79.2, 71.5, 53.1, 43.2, 42.7, 34.6, 31.7, 21.8. Visible peaks for minor isomer (**15d**): δ 128.4, 128.1, 127.7, 76.4, 75.2, 62.2, 45.9, 41.1, 38.4, 35.7. Anal. Calcd. for $C_{16}H_{19}ClHgO_3$: C, 38.79; H, 3.87. Found C, 38.67; H, 3.89.

Mercuric chlorides 14e and 15e. $Hg(OAc)_2$ (182 mg, 0.571 mmol) was added to a flame-dried flask containing norbornene **7e** (103 mg, 0.459 mmol) in THF (0.46 mL). The mixture was stirred at room temperature for 24 h, quenched with NaCl (202 mg, 3.45 mmol) and stirred for 12 h. After quenching with water (10 mL), the aqueous layer was extracted into CH_2Cl_2 (4×8 mL), and the combined organic layers were washed with brine (10 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=1:9) to give an inseparable mixture of **14e** and **15e** (165 mg, 0.318 mmol, 69%, **14e**:**15e**=4:1) as a white solid: R_f 0.63 (EtOAc:hexanes=1:4); IR (CH_2Cl_2): 2956 (s), 2885 (s), 2857 (s), 1732 (s), 1463 (m), 1444 (w), 1371 (s), 1301 (m), 1236 (s), 1160 (m), 1136 (m), 1098 (m), 1071 (m) cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 5.54 (d, 0.2H, J = 6.7 Hz), 4.89 (d, 0.8H, J = 6.7 Hz), 4.18 (dt, 0.2H, J = 9.6, 3.1 Hz), 4.13 (dt, 0.8H, J = 9.7, 3.7 Hz), 3.56 (dd, 0.8H, J = 7.0, 2.3 Hz), 2.95 (dd, 0.2H, J = 7.0, 2.4 Hz), 2.56 (dd, 0.2H, J = 8.7, 4.3 Hz), 2.51 (dd, 0.8H, J = 4.0, 1.3 Hz), 2.39 (d, 1H, J = 5.2 Hz), 2.045 (s, 2.4H), 2.039 (d, 0.6H), 1.97 (ddd, 0.2H, J = 13.2, 9.7, 4.4 Hz), 1.88 (ddd, 0.8H, J = 13.6, 9.7, 5.5 Hz), 1.61 (m, 0.8 H), 1.57 (m, 0.2H), 1.31 (m, 0.8H), 1.27 (m, 0.2H), 0.88 (s, 1.8H), 0.86 (s, 7.2H), 0.76 (dt, 1H, J = 13.5, 3.3 Hz), 0.07 (s, 0.6H), 0.023 (s, 0.6H), 0.017 (s, 2.4H), 0.011 (s, 2.4H). ^{13}C NMR ($CDCl_3$, 100 MHz); Major isomer (**14e**): δ 169.7, 80.1, 72.1, 53.5, 46.3, 43.4, 34.9, 34.7, 25.8, 21.8, 18.02, -4.8. Visible peaks for minor isomer (**15e**): δ 77.2, 75.3, 63.0, 49.3, 41.6, 41.3, 35.8, 25.8, 18.0, -4.98, -5.04. Anal. Calcd. for $C_{15}H_{27}ClHgO_3Si$: C, 34.68; H, 5.24. Found C, 34.79; H, 5.22.

Mercuric chlorides 14f and 15f. $Hg(OAc)_2$ (486 mg, 1.52 mmol) was added to a flame-dried flask containing norbornene **7f** (44.2 mg, 0.290 mmol) in THF (0.2 mL). The mixture was stirred at room temperature for 10 d, quenched with NaCl (141 mg, 2.41 mmol) and stirred for 12 h. After quenching with water (5 mL), the aqueous layer was extracted into CH_2Cl_2 (4×5 mL), and the combined organic layers were washed with brine (5 mL) and dried ($MgSO_4$). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography (EtOAc:hexanes=3:7) to give an inseparable mixture of **14f** and **15f** (63.5 mg, 0.142 mmol, 49%, **14f**:**15f**=9:1) as a white solid: R_f 0.37 (EtOAc:hexanes=3:7); IR (CH_2Cl_2): 3056 (w), 2976 (m), 2882 (w), 1716 (s), 1462 (w), 1440 (m), 1376 (s), 1248 (s), 1179 (w), 1072 (s), 1045 (s), 1020 (s) cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 5.37 (d, 0.11H, J = 7.0 Hz), 5.01 (dt, 0.11H, J = 10.0, 4.0 Hz), 4.93 (dt, 0.89H, J = 10.1, 3.9 Hz), 4.91 (d, 0.89H, J = 7.7 Hz), 3.28 (dd, 0.89H, J = 7.0, 2.4 Hz), 2.91 (dd, 0.11H, J = 7.0, 2.4 Hz), 2.85 (d, 0.89H, J = 2.7 Hz), 2.78 (d, 0.11H, J = 4.4 Hz), 2.66 (d, 0.11H, J = 3.6 Hz), 2.46 (d, 0.89H, J = 5.0 Hz), 2.07-2.04 (m, 1H), 2.04 (s, 3H), 2.02 (s, 3H), 1.71 (dt, 1H, J = 11.2, 1.5 Hz), 1.39 (d, 0.89H, J = 10.8 Hz), 1.23 (m, 0.11H), 0.97 (dt, 0.11H, J = 13.7, 3.4 Hz), 0.92 (dt, 0.89H, J = 14.1, 3.5 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz) for major isomer (**14f**): δ 170.8, 169.6, 79.4, 74.4, 53.3, 43.5, 42.7, 34.9, 31.6, 21.7, 21.0. Anal. Calcd. for $C_{11}H_{15}ClHgO_4$: C, 29.54; H, 3.38. Found C, 29.76; H, 3.50.

Cartesian coordinates (in Å) and total energies (in a.u.) predicted theoretically for the structures in Figures 4 to 8

FIGURE 4

OH-exo-**20**

SVWN/D95V, E_t =-346.004660674 a. u.

6	-1.278769	-1.111351	-0.469872
6	-1.832264	0.125575	-0.443605
6	-0.886882	1.025289	0.337074
6	0.030088	-1.034943	0.290536
6	-0.332850	0.014734	1.363286
6	1.006610	-0.198691	-0.590522
6	0.361568	1.213868	-0.570235
1	-1.678152	-2.012501	-0.942470
1	-2.778081	0.444274	-0.890627
1	0.473176	-1.986067	0.620501
1	-1.317166	1.959310	0.728557
1	0.537720	0.403718	1.932908
1	-1.096034	-0.347059	2.072060
1	1.104249	-0.618126	-1.603872
1	1.080257	1.933556	-0.133607
1	0.089754	1.577768	-1.574378
8	2.353336	-0.214934	-0.069750
1	2.352589	0.157702	0.848961

B3PW91/D95, E_t =-347.772273986 a. u.

6	-1.280471	-1.121306	-0.477645
6	-1.839102	0.111736	-0.472670
6	-0.905827	1.032688	0.320341
6	0.027451	-1.034209	0.310172
6	-0.368405	0.026711	1.377341
6	1.018306	-0.199292	-0.576819
6	0.375433	1.227849	-0.561002
1	-1.663817	-2.022030	-0.943817
1	-2.770942	0.419549	-0.934531
1	0.455143	-1.977128	0.653108
1	-1.348029	1.959611	0.690141
1	0.476430	0.418487	1.962279
1	-1.142104	-0.331050	2.062851
1	1.107947	-0.614411	-1.581470
1	1.070409	1.943423	-0.103073
1	0.134681	1.592223	-1.563435
8	2.386264	-0.227285	-0.072886
1	2.425869	0.164543	0.822732

OH-exo-**21**

SVWN/D95V, E_t =-346.004512895 a. u.

6	-1.284740	-1.089252	-0.507901
6	-1.834001	0.147872	-0.436090
6	-0.884569	1.015142	0.374939
6	0.025374	-1.041909	0.253624
6	-0.318708	-0.027095	1.362275
6	0.997183	-0.184715	-0.592070
6	0.363047	1.230962	-0.532406
1	-1.688393	-1.971306	-1.012423
1	-2.779766	0.485074	-0.870285
1	0.472792	-2.001553	0.549654
1	-1.306668	1.938823	0.798774
1	0.581867	0.321589	1.900088
1	-1.076295	-0.406403	2.068124
1	1.078176	-0.568473	-1.629512
1	1.073989	1.925261	-0.044611
1	0.090061	1.633147	-1.522514
8	2.279337	-0.247853	0.077636
1	2.938025	0.320627	-0.392608

B3PW91/D95, E_t =-347.774072565 a. u.

6	-1.277784	-1.122217	-0.490271
6	-1.841383	0.109019	-0.461427
6	-0.911328	1.019291	0.345941
6	0.030160	-1.038994	0.297318
6	-0.355444	0.002559	1.382134
6	1.007999	-0.178312	-0.581328
6	0.363849	1.234922	-0.540568
1	-1.620629	-1.993420	-1.038122
1	-2.737460	0.437053	-0.978032
1	-1.352341	1.939593	0.732748
1	0.455293	-1.988465	0.632714
1	-1.120734	-0.367701	2.071180
1	0.509125	0.380743	1.938308
1	1.087951	-0.583103	-1.599291
8	2.338209	-0.072421	0.015794
1	1.070977	1.919975	-0.061432
1	0.121499	1.620124	-1.534846
1	2.784226	-0.943045	-0.000376

OH-endo-**20**

SVWN/D95V, E_t =-346.007474382 a. u.

6	0.344024	1.473157	-0.038297
6	1.073931	0.805032	-0.969453
6	1.192375	-0.634867	-0.508211
6	-0.021328	0.471804	1.042108
6	1.219901	-0.438027	1.025100
6	-1.073093	-0.468751	0.366855
6	-0.221206	-1.266858	-0.656145
1	0.061596	2.529802	-0.045052
1	1.506931	1.208530	-1.889684
1	-0.350858	0.885526	2.005776
1	2.008494	-1.221776	-0.955652
1	1.078225	-1.384783	1.580881
1	2.129615	0.075438	1.380052
1	-1.546105	-1.126041	1.115566
1	-0.188193	-2.342914	-0.408135
1	-0.640144	-1.165055	-1.672394
8	-2.170295	0.247889	-0.227529
1	-1.784824	0.909224	-0.862868

B3PW91/D95, E_t =-347.774717612 a. u.

6	0.423383	1.478850	-0.071022
6	1.148209	0.767561	-0.970399
6	1.195556	-0.680177	-0.482367
6	-0.018277	0.508307	1.024822
6	1.199992	-0.452951	1.057706
6	-1.091785	-0.433953	0.364352
6	-0.250160	-1.260876	-0.662923
1	0.137722	2.523526	-0.131061
1	1.559919	1.118865	-1.911027
1	1.990520	-1.301121	-0.899099
1	-0.345406	0.953607	1.964956
1	2.112209	0.032169	1.418080
1	1.018894	-1.372086	1.629613
1	-1.548533	-1.075713	1.121952
8	-2.220773	0.269131	-0.216609
1	-0.270143	-2.330556	-0.424897
1	-0.632719	-1.137506	-1.681517
1	-1.897786	0.875202	-0.915155

OH-endo-**21**

SVWN/D95V, E_t =-346.001931075 a. u.

6	0.442517	1.455007	-0.172101
6	1.177205	0.676651	-1.003381
6	1.193656	-0.721353	-0.416343
6	-0.029174	0.572712	0.967890
6	1.163032	-0.395811	1.092549
6	-1.083799	-0.390207	0.370254
6	-0.255227	-1.270256	-0.603249
1	0.215076	2.518012	-0.275386
1	1.675665	0.974923	-1.929895
1	-0.372481	1.087377	1.876987
1	1.988596	-1.392274	-0.775866
1	0.950374	-1.279614	1.725811
1	2.079797	0.107968	1.441723
1	-1.506014	-1.014548	1.188739
1	-0.314566	-2.342455	-0.340268
1	-0.602392	-1.136102	-1.643849
8	-2.122392	0.389791	-0.249655
1	-2.784183	-0.202074	-0.684468

B3PW91/D95, E_t =-347.771100227 a. u.

6	0.464526	1.465664	-0.168313
6	1.196414	0.688693	-1.001150
6	1.202904	-0.724760	-0.422195
6	-0.023653	0.576228	0.974008
6	1.175174	-0.403628	1.099338
6	-1.089953	-0.391719	0.372925
6	-0.258485	-1.273824	-0.615501
1	0.157427	2.492940	-0.321552
1	1.617606	0.966098	-1.961591
1	1.988573	-1.391982	-0.781926
1	-0.360343	1.086922	1.876968
1	2.086501	0.090738	1.448290
1	0.965944	-1.280271	1.726699
1	-1.514194	-1.010123	1.179159
8	-2.150396	0.388872	-0.244255
1	-0.318250	-2.337908	-0.354976
1	-0.603159	-1.145078	-1.647344
1	-2.818494	-0.202236	-0.644366

OAc-exo-**20**

SVWN/D95V, E_t = -497.846385039 a.u.

6	-2.363734	-0.205751	-1.149542
6	-2.808748	0.598466	-0.153541
6	-1.888590	0.392802	1.038674
6	-1.148735	-0.944838	-0.618546
6	-1.535397	-1.099861	0.867631
6	-0.037915	0.120250	-0.497353
6	-0.532505	1.042585	0.639464
1	-2.779991	-0.321033	-2.153715
1	-3.666132	1.277057	-0.177825
1	-0.829314	-1.843232	-1.166187
1	-2.276564	0.712538	2.017149
1	-0.686688	-1.424712	1.497904
1	-2.401941	-1.766485	1.010847
1	0.168381	0.667041	-1.434204
1	0.188315	1.010337	1.477373
1	-0.631407	2.090816	0.317332
8	1.183590	-0.594962	-0.106134
6	2.338367	0.150357	-0.115367
8	2.352790	1.354205	-0.420992
6	3.512765	-0.681603	0.274117
1	4.419758	-0.061041	0.298245
1	3.344230	-1.142064	1.263007
1	3.647261	-1.507603	-0.446130

B3PW91/D95, E_t = -500.352475835 a u.

6	2.347684	0.031928	-1.215114
6	2.851801	-0.603659	-0.131464
6	1.975860	-0.228768	1.067780
6	1.131591	0.835448	-0.746078
6	1.592145	1.229263	0.685824
6	0.035524	-0.219559	-0.412346
6	0.599137	-0.947203	0.844835
1	2.712928	-0.001268	-2.235376
1	3.713557	-1.261138	-0.091670
1	0.781980	1.627380	-1.408755
1	2.413200	-0.391943	2.054103
1	0.785175	1.645162	1.299534
1	2.449344	1.908859	0.678496
1	-0.187552	-0.898321	-1.238758
1	-0.069817	-0.787051	1.697812
1	0.702785	-2.023546	0.688928
8	-1.202845	0.530424	-0.093184
6	-2.393515	-0.165950	-0.106086
8	-2.466278	-1.378081	-0.357576
6	-3.550269	0.741916	0.220813
1	-4.484606	0.181116	0.170803
1	-3.423553	1.161275	1.224744
1	-3.580205	1.580231	-0.482774

OAc-exo-**21**, SVWN/D95V

E_t = -497.836416335 a. u.

6	2.320972	0.062594	1.186714
6	2.758488	0.703102	0.075225
6	1.881983	0.247972	-1.080193
6	1.156679	-0.815338	0.768497
6	1.585140	-1.206500	-0.660186
6	-0.005531	0.149818	0.440474
6	0.487790	0.894543	-0.825093
1	2.713238	0.143846	2.203884
1	3.583560	1.416861	-0.002611
1	0.856250	-1.618617	1.456023
1	2.277895	0.413826	-2.092847
1	0.764887	-1.674505	-1.234671
1	2.481653	-1.847750	-0.670526
1	-0.241532	0.822209	1.286668
1	-0.200465	0.682216	-1.665495
1	0.556281	1.987160	-0.687427
8	-1.160731	-0.695094	0.145388
6	-2.424628	-0.149066	0.025984
8	-3.367461	-0.891852	-0.266720
6	-2.557026	1.324814	0.285675
1	-3.587235	1.627280	0.048706
1	-2.354900	1.557066	1.348217
1	-1.847296	1.914343	-0.321841

OAc-endo-**20**, SVWN/D95V

E_t = -497.846340456 a. u.

6	0.959117	-0.594216	-1.372726
6	0.953675	-1.217534	-0.694046
6	2.382514	-0.294530	0.428632
6	0.732901	0.749497	-0.709520
6	2.163155	1.080952	-0.238862
6	0.094509	0.445956	0.675248
6	1.200989	-0.287283	1.447442
1	0.345196	-1.005249	-2.178619
1	2.310669	-2.242033	-0.833604
1	0.180700	1.506899	-1.282730
1	3.368357	-0.488309	0.876577
1	2.208168	1.924113	0.477367
1	2.847561	1.266659	-1.083284
1	-0.229192	1.394170	1.145046
1	1.477006	0.252366	2.370405
1	0.870491	-1.303519	1.720837
8	-1.073292	-0.427951	0.579673
6	-2.200275	0.134925	0.032869
8	-2.247127	1.322264	-0.332286
6	-3.302927	-0.863777	-0.058202
1	-4.238714	-0.364412	-0.347688
1	-3.049281	-1.630865	-0.812403
1	-3.429545	-1.388266	0.903994

OAc-endo-**21**, SVWN/D95V

E_t = -497.833897748 a. u.

6	-1.590332	-1.453806	0.046149
6	-2.071259	-0.801230	-1.038925
6	-2.032579	0.682590	-0.726519
6	-1.231831	-0.403555	1.080198
6	-2.309487	0.661051	0.792448
6	0.009028	0.342957	0.539013
6	-0.523329	1.075133	-0.718075
1	-1.469792	-2.529989	0.184372
1	-2.426886	-1.237679	-1.975971
1	-1.115759	-0.755980	2.115111
1	-2.666059	1.331012	-1.349768
1	-2.119803	1.633845	1.287553
1	-3.322788	0.304190	1.039352
1	0.381517	1.060210	1.298793
1	-0.396249	2.170749	-0.636644
1	-0.004987	0.724097	-1.628616
8	1.042108	-0.638686	0.259349
6	2.335010	-0.246405	-0.027412
8	3.175973	-1.112872	-0.288855
6	2.627200	1.227570	0.018996
1	3.666295	1.384358	-0.304522
1	1.944698	1.799593	-0.634770
1	2.510648	1.622235	1.045915

$OSiH_3$-exo-**20**, SVWN/D95V

E_t = -635.824943834 a. u.

6	1.683939	1.362325	-0.487143
6	2.584303	0.349810	-0.444235
6	1.956962	-0.782075	0.352090
6	0.460945	0.898965	0.281390
6	1.113853	0.018639	1.366451
6	-0.206901	-0.211243	-0.585476
6	0.826104	-1.354340	-0.549747
1	1.793453	2.334767	-0.974588
1	3.582505	0.327054	-0.891210
1	-0.241508	1.683399	0.609042
1	2.647118	-1.539055	0.753200
1	0.375631	-0.604573	1.904200
1	1.728205	0.600682	2.073690
1	-0.421324	0.160293	-1.610788
1	0.333091	-2.225286	-0.081957
1	1.189832	-1.643008	-1.549175
8	-1.425318	-0.691825	0.025915
14	-2.872160	0.234278	-0.000415
1	-3.137055	0.719450	-1.406550
1	-3.950304	-0.692137	0.467587
1	-2.802086	1.440632	0.905068

OSiH$_3$-exo-**21**, SVWN/D95V

E_t = -635.824264968 a. u.

6	-2.129825	-0.942126	-0.704766
6	-2.557988	0.339954	-0.603066
6	-1.644322	1.044696	0.385318
6	-0.932951	-1.086726	0.215889
6	-1.317432	-0.114818	1.349298
6	0.220883	-0.282648	-0.432586
6	-0.275499	1.185643	-0.343613
1	-2.548832	-1.739660	-1.324222
1	-3.400255	0.805087	-1.123644
1	-0.623232	-2.105178	0.490284
1	-2.024941	1.978677	0.825218
1	-0.465859	0.099094	2.020752
1	-2.194534	-0.456842	1.923657
1	0.411175	-0.605190	-1.478701
1	0.436664	1.768358	0.272580
1	-0.374219	1.674943	-1.326993
8	1.402289	-0.501721	0.369321
14	2.943568	0.074211	-0.119348
1	3.019834	1.582176	-0.082350
1	3.919326	-0.513359	0.851223
1	3.239410	-0.377138	-1.530343

OSiH$_3$-endo-**20**, SVWN/D95V

E_t = -635.825027583 a. u.

6	-0.475553	1.258319	-0.732365
6	-0.996755	1.451341	0.506850
6	-1.726397	0.179967	0.894525
6	-0.859445	-0.141003	-1.166662
6	-2.236916	-0.284008	-0.489001
6	-0.035877	-1.125176	-0.272865
6	-0.626981	-0.891022	1.142484
1	0.113121	1.964286	-1.324579
1	-0.918572	2.347315	1.129214
1	-0.785228	-0.362429	-2.241122
1	-2.467638	0.273575	1.702219
1	-2.619447	-1.322994	-0.483075
1	-2.993048	0.393858	-0.920004
1	-0.233268	-2.158433	-0.612728
1	-1.062307	-1.820839	1.549068
1	0.148219	-0.542203	1.849030
8	1.381883	-0.982164	-0.361862
14	2.381942	0.313299	0.146680
1	2.003531	0.842018	1.509396
1	3.747244	-0.306779	0.202768
1	2.412690	1.473242	-0.816601

OSiH$_3$-endo-**21**, SVWN/D95V

E_t = -635.821908589 a. u.

6	-1.322008	1.409830	0.333464
6	-1.802460	0.505766	1.221401
6	-1.816536	-0.843519	0.530458
6	-1.016860	0.659649	-0.948303
6	-2.119354	-0.416575	-0.922464
6	0.217794	-0.225225	-0.647969
6	-0.318921	-1.255301	0.382386
1	-1.171228	2.481103	0.481658
1	-2.126568	0.688078	2.249759
1	-0.907949	1.267700	-1.858084
1	-2.461273	-1.614822	0.978249
1	-1.961753	-1.230187	-1.657690
1	-3.128199	0.011973	-1.044032
1	0.540302	-0.740369	-1.581785
1	-0.220822	-2.293204	0.014880
1	0.224993	-1.167532	1.340722
8	1.291957	0.593679	-0.160999
14	2.857142	-0.038201	0.142213
1	3.382945	-0.741698	-1.088405
1	3.706907	1.144543	0.485168
1	2.857073	-1.027959	1.282727

OCH$_3$-exo-**20**, SVWN/D95V

E_t = -385.082205415 a. u.

6	1.358497	1.323647	-0.481394
6	2.201874	0.262317	-0.469421
6	1.527910	-0.841303	0.328930
6	0.127804	0.922165	0.308418
6	0.751284	-0.007093	1.368366
6	-0.615740	-0.137379	-0.564470
6	0.348237	-1.339103	-0.553806
1	1.512985	2.293921	-0.961316
1	3.187433	0.188959	-0.938460
1	-0.515650	1.744131	0.660725
1	2.182418	-1.640544	0.707437
1	-0.010232	-0.595304	1.913648
1	1.410951	0.529682	2.070807
1	-0.819600	0.262687	-1.583181
1	-0.183029	-2.184671	-0.080620
1	0.674256	-1.642248	-1.561677
8	-1.852721	-0.573648	0.037885
6	-2.884117	0.418616	-0.012776
1	-3.041863	0.784404	-1.052267
1	-3.809861	-0.059086	0.346672
1	-2.660530	1.296045	0.632077

OCH$_3$-exo-**21**, SVWN/D95V

E_t = -385.081547832 a. u.

6	-1.714782	-0.964289	-0.691581
6	-2.165584	0.310302	-0.593474
6	-1.258635	1.035533	0.386399
6	-0.510293	-1.082851	0.222634
6	-0.907910	-0.113360	1.354449
6	0.622379	-0.262799	-0.438976
6	0.105388	1.198290	-0.347605
1	-2.122540	-1.772527	-1.304687
1	-3.019137	0.757613	-1.111311
1	-0.182536	-2.094994	0.499855
1	-1.653908	1.964695	0.823904
1	-0.058271	0.119907	2.021967
1	-1.777168	-0.468780	1.932592
1	0.811440	-0.584105	-1.487558
1	0.807872	1.790051	0.271551
1	-0.004367	1.691996	-1.327473
8	1.811315	-0.475856	0.350943
6	2.970117	0.133982	-0.226007
1	2.877886	1.241828	-0.280867
1	3.828494	-0.122838	0.415396
1	3.157632	-0.244844	-1.255944

OCH$_3$-endo-**20**, SVWN/D95V

E_t = -385.080063410 a. u.

6	0.462936	1.454428	-0.314638
6	1.445008	0.824011	-1.003425
6	1.754207	-0.466874	-0.270065
6	0.119605	0.583579	0.875372
6	1.496999	-0.034082	1.188953
6	-0.592207	-0.689033	0.304488
6	0.519695	-1.392024	-0.493415
1	-0.007983	2.411763	-0.554136
1	1.938817	1.161269	-1.918856
1	-0.411671	1.070393	1.707963
1	2.723704	-0.935612	-0.496220
1	1.446212	-0.889148	1.891645
1	2.219790	0.714435	1.555646
1	-0.946003	-1.306423	1.165120
1	0.712537	-2.412826	-0.119468
1	0.220055	-1.451768	-1.553421
8	-1.695573	-0.421256	-0.571434
6	-2.744989	0.305499	0.075810
1	-2.421343	1.330263	0.362716
1	-3.577428	0.381095	-0.641939
1	-3.099621	-0.216417	0.993938

OCH$_3$-endo-**21**, SVWN/D95V

E_t = -385.077799438 a. u.

6	-0.421373	1.392919	-0.514111
6	-1.097150	1.274753	0.656446
6	-1.512294	-0.178034	0.788356
6	-0.385601	0.023467	-1.161353
6	-1.750272	-0.532079	-0.697610
6	0.529194	-0.921935	-0.309188
6	-0.204003	-0.977463	1.057502
1	0.024400	2.299523	-0.933720
1	-1.314554	2.061686	1.383992
1	-0.156869	-0.008324	-2.236981
1	-2.331329	-0.386754	1.492910
1	-1.869171	-1.618258	-0.876272
1	-2.599360	0.018964	-1.136289
1	0.512524	-1.917878	-0.788797
1	-0.418774	-2.021848	1.343545
1	0.398876	-0.523893	1.865307
8	1.932201	-0.629112	-0.264855
6	2.330638	0.626801	0.293406
1	1.849497	0.831724	1.274152
1	3.423888	0.570195	0.427238
1	2.088426	1.477192	-0.376932

OCH$_3$-endo-**22**, SVWN/D95V

E_t = -385.078876208 a. u.

6	0.974504	1.402926	-0.325750
6	1.502587	0.483800	-1.169923
6	1.452816	-0.857689	-0.466022
6	0.573596	0.670367	0.940437
6	1.664221	-0.417310	0.998910
6	-0.646336	-0.206760	0.570525
6	-0.056728	-1.251591	-0.415598
1	0.847747	2.474286	-0.495045
1	1.897783	0.651452	-2.175668
1	0.413038	1.288845	1.835304
1	2.116465	-1.641470	-0.861722
1	1.448183	-1.220495	1.730619
1	2.667509	0.002617	1.181787
1	-1.035267	-0.713584	1.486260
1	-0.190199	-2.286707	-0.052087
1	-0.530468	-1.163081	-1.410583
8	-1.675946	0.626464	0.020213
6	-2.890943	-0.089179	-0.221642
1	-3.281592	-0.558046	0.710459
1	-3.628364	0.639004	-0.595855
1	-2.759561	-0.891912	-0.980790

CH_2OH-exo-**20**, SVWN/D95V

E_t = -385.090171063 a. u.

6	1.739858	1.118050	0.057418
6	2.223722	-0.101486	-0.289364
6	1.143711	-1.119554	0.022863
6	0.335314	0.903604	0.587471
6	0.488831	-0.474645	1.260962
6	-0.513201	0.526750	-0.673610
6	0.008971	-0.891534	-1.021359
1	2.204782	2.092716	-0.120610
1	3.166589	-0.320022	-0.800354
1	-0.101350	1.716311	1.190428
1	1.468519	-2.167493	0.114530
1	-0.489565	-0.919400	1.513302
1	1.165481	-0.445125	2.132423
1	-0.291912	1.244890	-1.487892
1	-0.796653	-1.631226	-0.853899
1	0.370692	-0.975823	-2.060389
6	-2.011097	0.575580	-0.452226
1	-2.295668	1.594745	-0.105726
1	-2.526391	0.376490	-1.419007
8	-2.377278	-0.420095	0.532436
1	-3.352956	-0.425892	0.684773

CH_2OH-exo-**21**, SVWN/D95V

E_t = -385.088911423 a. u.

6	-1.733247	-0.898247	-0.757046
6	-2.150432	0.383092	-0.604361
6	-1.247717	1.031176	0.428994
6	-0.553317	-1.097756	0.176384
6	-0.969120	-0.177745	1.345091
6	0.617893	-0.272721	-0.446009
6	0.145516	1.190083	-0.248519
1	-2.148824	-1.663268	-1.418813
1	-2.979080	0.879199	-1.117969
1	-0.295145	-2.141980	0.417988
1	-1.631351	1.946831	0.904551
1	-0.160575	0.007913	2.078441
1	-1.873620	-0.538726	1.863729
1	0.736253	-0.514586	-1.518214
1	0.854537	1.729524	0.407211
1	0.086760	1.745791	-1.198671
6	1.933949	-0.551611	0.241305
1	2.217552	-1.617684	0.089565
1	1.826761	-0.372089	1.336799
8	2.912109	0.339827	-0.338307
1	3.808713	0.182841	0.046811

CH_2OH-endo-**21**, SVWN/D95V

E_t = -385.092315279 a. u.

6	-0.454961	-1.418945	-0.427437
6	-1.453306	-0.747222	-1.054402
6	-1.768629	0.478148	-0.218894
6	-0.110653	-0.634980	0.824790
6	-1.497213	-0.071797	1.196012
6	0.590661	0.688144	0.358851
6	-0.546927	1.434431	-0.382035
1	0.020449	-2.349884	-0.752199
1	-1.953412	-1.018659	-1.988592
1	0.428152	-1.178518	1.618203
1	-2.746001	0.951106	-0.398417
1	-1.452004	0.719152	1.968814
1	-2.210990	-0.858381	1.494720
1	0.905287	1.241440	1.265108
1	-0.755097	2.416548	0.078936
1	-0.304135	1.604742	-1.448173
6	1.806658	0.450850	-0.511262
1	1.480546	-0.020726	-1.466591
1	2.310057	1.403536	-0.753543
8	2.809198	-0.346147	0.155977
1	2.409792	-1.212958	0.420176

CH_2OH-endo-**22**, SVWN/D95V

E_t = -385.091805872 a. u.

6	-0.515977	-1.434914	-0.380180
6	-1.506103	-0.756286	-1.012330
6	-1.770319	0.504179	-0.210505
6	-0.125469	-0.624152	0.838796
6	-1.486996	-0.006911	1.216865
6	0.604489	0.653712	0.313370
6	-0.523156	1.415343	-0.432634
1	-0.064950	-2.387613	-0.670882
1	-2.031737	-1.041497	-1.928304
1	0.429423	-1.164156	1.619617
1	-2.735281	1.002473	-0.389529
1	-1.407396	0.807924	1.962690
1	-2.218900	-0.760391	1.554505
1	0.940283	1.241482	1.195521
1	-0.687051	2.422200	-0.007551
1	-0.298103	1.534868	-1.509219
6	1.801231	0.359663	-0.562921
1	1.485886	-0.255309	-1.426293
1	2.231704	1.308624	-0.955750
8	2.801041	-0.426951	0.123088
1	3.081596	0.043204	0.947717

CH$_2$OH-endo-**23**, SVWN/D95V

E_t = -385.091280933 a. u.

6	1.041460	1.353330	-0.443736
6	1.531702	0.343923	-1.205922
6	1.428702	-0.927456	-0.384560
6	0.614393	0.750583	0.880839
6	1.667942	-0.365212	1.032065
6	-0.652657	-0.120444	0.607168
6	-0.096225	-1.253389	-0.299920
1	0.960140	2.410104	-0.713714
1	1.931249	0.407370	-2.222072
1	0.497230	1.453597	1.720127
1	2.057760	-1.770096	-0.709372
1	1.424518	-1.087608	1.834412
1	2.689992	0.027911	1.167310
1	-1.002981	-0.545375	1.568749
1	-0.263167	-2.252392	0.141740
1	-0.552682	-1.247122	-1.310864
6	-1.802487	0.642188	-0.014526
1	-1.470702	1.074849	-0.985427
1	-2.132112	1.469249	0.639894
8	-2.974883	-0.187086	-0.180217
1	-2.737160	-0.984940	-0.717489

CH$_2$OH-endo-**24**, SVWN/D95V

E_t = -385.084740163 a. u.

6	0.462130	1.317109	0.662532
6	1.105159	1.313128	-0.529822
6	1.494916	-0.121617	-0.821937
6	0.426371	-0.115440	1.159573
6	1.771491	-0.632619	0.606923
6	-0.538629	-0.934968	0.245626
6	0.148661	-0.854584	-1.140654
1	0.039483	2.175754	1.188889
1	1.315156	2.168754	-1.176831
1	0.235588	-0.252753	2.236528
1	2.284120	-0.271660	-1.574610
1	1.876646	-1.733650	0.667416
1	2.641929	-0.139306	1.072310
1	-0.512519	-1.983225	0.611750
1	0.328559	-1.857804	-1.568802
1	-0.462668	-0.262235	-1.844194
6	-1.991437	-0.519045	0.265689
1	-2.594051	-1.287798	-0.270430
1	-2.343094	-0.481119	1.322362
8	-2.126432	0.768640	-0.373024
1	-3.069666	1.064135	-0.367768

FIGURE 5

C_2H_4, D_{2h}

B3PW91/D95

E_t = -78.5476784512 a. u.

6	0.000000	0.000000	0.672805
6	0.000000	0.000000	-0.672805
1	0.000000	0.925168	-1.245611
1	0.000000	-0.925168	-1.245611
1	0.000000	0.925168	1.245611
1	0.000000	-0.925168	1.245611

$Hg(O_2CH)_2$, D_{2d}

B3PW91/LanL2DZ,

E_t = -420.912796548 a. u.

80	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.711145
6	0.000000	0.000000	-2.711145
8	0.000000	1.129388	2.079104
8	0.000000	-1.129388	2.079104
8	1.129388	0.000000	-2.079104
8	-1.129388	0.000000	-2.079104
1	0.000000	0.000000	3.805139
1	0.000000	0.000000	-3.805139

pre-reaction complex, C_2

B3PW91/LanL2DZ,

E_t = -499.470191909 a. u.

80	0.000000	0.000000	0.373385
8	-1.035551	1.995645	1.147511
6	-0.620120	0.274778	-2.437335
6	0.620120	-0.274778	-2.437335
8	1.035551	-1.995645	1.147511
6	0.000000	2.701433	0.819481
8	1.044430	2.170536	0.274818
6	0.000000	-2.701433	0.819481
8	-1.044430	-2.170536	0.274818
1	-0.016093	3.780463	1.007556
1	0.016093	-3.780463	1.007556
1	-0.762052	1.353494	-2.462438
1	0.762052	-1.353494	-2.462438
1	-1.515805	-0.343891	-2.456939
1	1.515805	0.343891	-2.456939

TS, C_s

B3PW91/LanL2DZ

E_t =-499.437829241 a. u.

80	-0.280734	-0.121209	0.000066
8	-2.365237	0.194052	1.132273
6	1.294916	-1.865891	0.002658
6	2.620445	-1.347015	-0.001662
8	3.084623	0.585949	0.000895
6	-2.983186	0.290638	-0.000151
8	-2.365069	0.188589	-1.132142
6	2.363561	1.656989	0.000344
8	1.080698	1.739701	-0.002875
1	-4.065177	0.464144	-0.000957
1	2.925683	2.604764	0.003163
1	0.963993	-2.353401	-0.916545
1	0.968606	-2.351022	0.924667
1	3.201955	-1.370176	-0.918392
1	3.209097	-1.372230	0.910406

product, C_1

B3PW91/LanL2DZ

E_t = -499.466101305 a. u.

80	-0.672804	0.542325	-0.355244
8	-2.599486	-0.584289	-0.945301
6	1.274769	1.615454	-0.412487
6	2.352355	0.954066	0.441924
8	2.850854	-0.330161	-0.129579
6	-3.279613	-0.256638	0.121496
8	-2.787030	0.480332	1.045425
6	2.084304	-1.441894	-0.033973
8	0.938865	-1.495553	0.444991
1	-4.304053	-0.639907	0.203652
1	2.619199	-2.303374	-0.445644
1	1.065810	2.615306	-0.010923
1	1.599153	1.720002	-1.453307
1	2.010699	0.755661	1.464245
1	3.266319	1.555847	0.478846

FIGURES 6-8

Reagent, norbornene

B3PW91/D95,

E_t = -272.594210763 a. u.

6	0.221366	0.245530	1.133578
6	0.221366	0.245530	-1.133578
6	-1.131925	0.792053	0.677390
6	-1.131925	0.792053	-0.677390
6	1.135937	0.788858	0.000000
6	0.221366	-1.287007	0.782377
6	0.221366	-1.287007	-0.782377
1	0.508943	0.471938	2.162278
1	0.508943	0.471938	-2.162278
1	-1.928730	1.113840	1.339661
1	-1.928730	1.113840	-1.339661
1	1.210048	1.881098	0.000000
1	2.140380	0.346009	0.000000
1	1.121767	-1.770567	1.181107
1	-0.649841	-1.798791	1.203719
1	1.121767	-1.770567	-1.181107
1	-0.649841	-1.798791	-1.203719

PRC-norbornene

B3PW91/LanL2DZ

E_t = -693.521794543 a. u.

6	-0.239523	1.973556	1.137642
6	-0.239523	1.973556	-1.137642
6	0.906907	1.076629	0.685853
6	0.906907	1.076629	-0.685853
6	-1.269358	1.739390	0.000000
6	0.233611	3.434241	0.781695
6	0.233611	3.434241	-0.781695
1	-0.582317	1.841260	2.163477
1	-0.582317	1.841260	-2.163477
1	1.684573	0.687086	1.336959
1	1.684573	0.687086	-1.336959
1	-1.706051	0.734359	0.000000
1	-2.079996	2.475589	0.000000
1	-0.481886	4.160652	1.182845
1	1.216184	3.662646	1.206467
1	-0.481886	4.160652	-1.182845
1	1.216184	3.662646	-1.206467
80	0.063339	-1.517411	0.000000
6	-0.108408	-2.128393	2.675465
6	-0.108408	-2.128393	-2.675465
8	-1.178349	-1.767302	2.045063
8	1.041831	-2.212161	2.089583
8	-1.178349	-1.767302	-2.045063
8	1.041831	-2.212161	-2.089583
1	-0.178869	-2.370820	3.742277
1	-0.178869	-2.370820	-3.742277

TS-norbornene

B3PW91/LanL2DZ

E_t = -693.489561363 a. u.

6	1.209844	-0.972482	-0.794708
6	1.880869	0.273699	-0.834381
6	2.872958	0.302301	0.297246
6	1.878784	-1.749950	0.362536
6	2.179967	-0.595717	1.353457
6	3.326214	-2.089983	-0.128085
6	4.004453	-0.683027	-0.202352
1	0.899447	-1.470548	-1.715549
1	1.942882	0.937608	-1.688372
1	3.215451	1.290929	0.595513
1	1.323207	-2.605457	0.749801
1	1.289822	-0.127872	1.788314
1	2.857231	-0.892807	2.160587
1	3.831855	-2.738350	0.596909
1	3.319675	-2.608805	-1.092456
1	4.858324	-0.608113	0.479681
1	4.362879	-0.431827	-1.206202
80	-0.953042	-0.125187	-0.128574
8	-2.751537	-0.707281	1.343664
6	-3.601699	-0.614718	0.372121
8	-3.241540	-0.303217	-0.830263
1	-4.661347	-0.806297	0.576191
8	0.368116	1.746129	-0.110796
6	0.518477	3.036113	0.219980
8	1.600292	3.653398	0.174878
1	-0.417879	3.526878	0.546734

product-norbornene

B3PW91/LanL2DZ

E_t = -693.519877594 a. u.

6	0.461566	-0.817354	-0.799235
6	1.159977	0.519543	-0.469815
6	2.236753	0.126007	0.563819
6	1.221867	-1.849225	0.077588
6	1.539411	-1.015603	1.343243
6	2.643056	-2.024309	-0.533975
6	3.329891	-0.652519	-0.220488
1	0.486034	-1.056061	-1.867690
1	1.576287	1.043427	-1.335825
1	0.694763	-2.792859	0.234890
1	2.618620	0.971709	1.138168
1	2.215995	-1.528042	2.035506
1	0.649152	-0.688667	1.892503
1	3.171000	-2.854048	-0.048267
1	4.218098	-0.786509	0.406281
1	3.647533	-0.118942	-1.123644
1	2.602472	-2.243408	-1.607099
80	-1.691417	-0.578824	-0.259822
8	0.142948	1.453073	0.134887
8	-3.621464	-0.669214	1.098325
6	-4.410133	-0.257033	0.149214
8	-3.973253	0.027423	-1.026384
1	-5.478926	-0.153676	0.373649
6	0.454106	2.789299	0.217180
8	1.510057	3.302607	-0.158070
1	-0.389304	3.329005	0.664134

PRC-OH-exo-**20**

B3PW91/LanL2DZ

E_t = -768.6973099 a. u.

6	-1.459161	0.424692	-0.997630
6	-1.315997	-0.936197	-0.949198
6	-2.220612	-1.445878	0.172638
6	-2.455584	0.815509	0.087838
6	-2.148991	-0.256507	1.168795
6	-3.848099	0.294663	-0.441597
6	-3.681810	-1.260313	-0.372203
1	-1.097832	1.092138	-1.774697
1	-0.806811	-1.567238	-1.671934
1	-1.996297	-2.440021	0.558386
1	-2.471352	1.862599	0.386457
1	-1.171468	-0.129955	1.645379
1	-2.905534	-0.317766	1.961052
1	-4.054405	0.653503	-1.451007
8	-4.964236	0.804127	0.333421
1	-4.410767	-1.684037	0.328701
1	-3.832071	-1.745685	-1.340378
80	1.184991	0.070070	-0.020831
8	0.966908	2.164735	1.154172
6	1.392975	2.804086	0.115085
8	1.720163	2.196204	-0.980547
1	1.479430	3.895679	0.159432
8	1.629053	-1.890087	1.298247
6	2.034394	-2.527797	0.248741
8	2.049089	-1.982381	-0.924615
1	2.375296	-3.563886	0.356112
1	-4.897959	0.524772	1.268759

PRC-OH-exo-**21**

B3PW91/LanL2DZ

E_t = -768.699668 a. u.

6	-1.425739	0.472326	-0.959967
6	-1.343836	-0.893737	-1.029427
6	-2.265785	-1.458097	0.049362
6	-2.401621	0.806184	0.164586
6	-2.146308	-0.366677	1.147013
6	-3.817349	0.388422	-0.389766
6	-3.718206	-1.159990	-0.471519
1	-1.041517	1.185110	-1.684670
1	-0.853461	-1.481436	-1.800016
1	-2.091048	-2.492744	0.342741
1	-2.354369	1.821197	0.561166
1	-1.164124	-0.330349	1.631247
1	-2.922447	-0.446293	1.913452
1	-4.019240	0.856554	-1.362560
8	-4.880396	0.709989	0.551144
1	-4.465405	-1.589057	0.202564
1	-3.893672	-1.546981	-1.478848
80	1.166169	0.059465	-0.009544
8	1.039113	2.190638	1.109558
6	1.491702	2.788720	0.056646
8	1.795488	2.145340	-1.024343
1	1.622811	3.876847	0.079334
8	1.627231	-1.878849	1.319065
6	1.986142	-2.546910	0.270409
8	1.972522	-2.027525	-0.913646
1	2.311832	-3.586340	0.391983
1	-5.008574	1.678084	0.608876

PRC-OH-endo-**20**

B3PW91/LanL2DZ

E_t = -768.698560174 a. u.

6	-0.932669	0.278900	-0.793634
6	-0.750647	-1.045951	-0.490559
6	-1.523337	-1.328253	0.793503
6	-1.831859	0.869950	0.286322
6	-1.401112	0.039767	1.523364
6	-3.255632	0.237678	0.032155
6	-3.038623	-1.271770	0.378850
1	-0.653907	0.783771	-1.714516
1	-0.286933	-1.799839	-1.120233
1	-1.232143	-2.222715	1.343895
1	-1.839587	1.955126	0.373696
1	-0.390565	0.277666	1.871353
1	-2.093374	0.132704	2.367517
1	-3.980729	0.705366	0.701928
8	-3.799005	0.483503	-1.287762
1	-3.670971	-1.585371	1.215771
1	-3.271092	-1.918880	-0.473824
80	1.822580	0.157660	-0.084282
8	1.621839	2.206494	1.172110
6	1.868148	2.893209	0.105280
8	2.087109	2.329668	-1.039834
1	1.891059	3.986928	0.168193
8	2.802372	-1.740467	0.967755
6	2.886865	-2.374449	-0.158469
8	2.471987	-1.859828	-1.268619
1	3.322517	-3.380075	-0.164125
1	-3.266451	0.023965	-1.968356

PRC-OH-endo-**21**

B3PW91/LanL2DZ

E_t = -768.698349107 a. u.

6	-0.960167	0.334914	-0.821326
6	-0.742262	-0.996529	-0.581039
6	-1.469896	-1.350482	0.711828
6	-1.832262	0.860398	0.313661
6	-1.352569	-0.016263	1.500038
6	-3.239439	0.222684	0.068606
6	-2.997026	-1.300427	0.330856
1	-0.757194	0.873672	-1.740387
1	-0.319815	-1.718814	-1.273607
1	-1.149379	-2.264556	1.210923
1	-1.854076	1.940234	0.449820
1	-0.338497	0.226297	1.832760
1	-2.022113	0.026156	2.366538
1	-3.953299	0.637711	0.794548
8	-3.661762	0.545359	-1.282997
1	-3.607185	-1.672036	1.161745
1	-3.220130	-1.897192	-0.559878
80	1.759718	0.148740	-0.127427
8	1.652116	2.159297	1.218682
6	1.900966	2.877884	0.173846
8	2.083233	2.354275	-0.995940
1	1.960324	3.967501	0.278386
8	2.530134	-1.839845	0.988805
6	2.863054	-2.371646	-0.142182
8	2.694993	-1.758591	-1.268686
1	3.302544	-3.376068	-0.145689
1	-4.569907	0.225072	-1.450666

PRC-OAc-exo-**20**

B3PW91/LanL2DZ, E_t = -921.277026512 a. u.

6	0.148872	0.030985	-1.051382
6	0.447381	-1.218256	-0.576724
6	-0.435661	-1.460112	0.646369
6	-0.928831	0.614308	-0.140112
6	-0.546818	-0.021614	1.222958
6	-2.210597	-0.212668	-0.482909
6	-1.884465	-1.635408	0.063322
1	0.459348	0.462898	-1.998181
1	1.057937	-1.970346	-1.068534
1	-1.080599	1.691342	-0.180502
1	-0.119059	-2.253812	1.322997
1	-1.338014	0.080098	1.971281
1	0.387554	0.375683	1.631511
1	-2.465497	-0.211396	-1.545829
1	-2.586031	-1.899838	0.861064
1	-1.944652	-2.403705	-0.711176
8	-3.323435	0.415261	0.255315
6	-4.609569	0.076538	-0.130292
8	-4.843130	-0.733374	-1.038002
6	-5.628602	0.819782	0.689767
1	-6.633395	0.526238	0.383496
1	-5.485157	0.603865	1.753609
1	-5.500886	1.899036	0.555210
80	2.808405	0.288239	-0.044653
8	2.219281	2.385459	0.996118
6	2.553426	3.021053	-0.078441
8	2.999160	2.409581	-1.129073
8	3.822518	-1.710408	-0.971911
6	4.161686	-2.088565	0.216312
8	3.873418	-1.391229	1.268723
1	2.455445	4.112258	-0.104643
1	4.708722	-3.029759	0.342958

5-coordinated-Hg-OH-endo-**21** complex

B3PW91/LanL2DZ, E_t = -768.677684 a. u.

6	-1.050327	-0.131504	-0.880237
6	-0.664522	-1.087252	0.026971
6	-1.532383	-0.905680	1.266301
6	-2.165452	0.682872	-0.233282
6	-1.754518	0.633189	1.262103
6	-3.397644	-0.280770	-0.201213
6	-2.963110	-1.386667	0.814294
1	-0.806616	-0.106364	-1.937627
1	-0.009157	-1.934642	-0.155688
1	-1.165527	-1.366928	2.183061
1	-2.380055	1.653577	-0.678107
1	-0.856134	1.218629	1.483415
1	-2.555825	0.948343	1.939791
1	-4.275312	0.269416	0.166979
8	-3.640118	-0.757861	-1.550869
1	-3.635396	-1.434857	1.678041
1	-2.934083	-2.372700	0.339038
80	1.565009	0.534163	-0.125469
8	1.280818	2.588429	1.083880
6	1.509959	3.266895	0.006129
8	1.758645	2.688958	-1.124194
1	1.491558	4.361166	0.050197
8	2.459422	-1.436319	-0.112613
6	3.753154	-1.808932	-0.069283